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The method of identifying mathematical model of industrial process of polymerization

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Abstract

The work presents identification method, allowing receiving a mathematical model of industrial processes of polymerization according to data of regular maintenance taking into account interference correlation. The method for receiving optimum estimates of model parameters, which can be employed to control the process, has been suggested. One of the widespread polymer plastic materials is polystyrene, obtained by continuous polymerization of styrol. Most industrious processes of polymerization are realized in the cascade of continuously operating reactors with stirring device.

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1. Introduction

One of the widespread polymer plastic materials is polystyrene, obtained by continuous polymerization of styrol. Most industrious processes of polymerization are realized in the cascade of continuously operating reactors with stirring device.

Development of mathematical models of processes in conditions of industrial production is connected with considerable difficulties. It is connected with the presence of different factors, taking place in industrial conditions, such as failure of ideality of reactors' interfusion, viscosity growth of polymerizing mass according to conversion growth and transition from one reactor to another, adherence of polymerizing mass at the surface of apparatus, change in density of polymerizing mass (Yılmaz & Orhan, 2010; Peltokorpi & Määttä, 2011; Ozcan, 2011).

2. State of problem

Insert The analysis of real conditions of industrial production of many processes of chemical technology has allowed to establish that these processes are greatly sensitive to various chance factors, influencing on the process, for instance, while using different sources of raw material supply the process characteristics vary. Meanwhile the process behaves itself as non-stationary one, that causes a necessity of its consideration.

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The task, to develop a mathematical model of industrial process is set, which considers an impact of various chance factors on it.

In many cases, there is a determinate mathematical model of the process, composed on the basis of the analysis of physico-chemical laws of the process.

The determinate mathematical model of industrial processes in the statics can be presented as

$$y_j = y_{j-1} + Ax_j \quad (1)$$

A dynamic linear model of the process in a discrete form will correspondingly be written:

$$y_{jn+1} = \theta_{1j} y_{jn} + \theta_{2j} y_{j-1n} + Ax_{jn} \quad (2)$$

These equations describe average idealized state of the process.

On the basis of stochastic approach a range of nonobservable variables, characterizes an impact of chance factors, unaccounted while constructing posterior determinate model is included into posterior determinate model of the process. The adequacy of the received stochastic model the polymerization process is estimated to minimum of the set criterion. Meanwhile additive correlated interference, taking into account deviate of determinate model from the real process is included into the model. Continuity of industrial process, character of unaccounted factors give ground to assume that all disturbing influences have a smooth character of change in time, their values in the following moment of time depend on values in the following moment, that is correlation in time of nonobservable noise in the object is observed, as evidenced by statistic researches of industrial processes.

Unaccounted factors can be considered as total unobservable noise in the object ε , which follows Gaussian law according to the limiting theorem and are chance sequences of non-controlled disturbances with zero mathematical expectation and unit variance, non-correlated between each other and in time.

Noise model in autoregressive form will be written as the following equation:

$$v_n = \lambda v_{n-1} + \tilde{b} \varepsilon_n \quad (3)$$

Stochastic model of the process dynamics in $(n+1)$ – the moment of the time considering operation of correlated interference takes the form of:

$$y_{jn+1} = \theta y_{jn} + (1-\theta) y_{j-1n} + A_j x_{jn} + v_{jn+1} \quad (4)$$

Stochastic model of the process with correlated interferences:

$$y_{jn+1} = (\theta + \lambda_j) y_{jn} + (1-\theta) y_{j-1n} - \theta \lambda_j y_{jn-1} - (1-\theta) \lambda_j y_{j-1n-1} + A_j x_{jn} - A_j \lambda_j x_{jn-1} + \tilde{b} \varepsilon_{jn} \quad (5)$$

This expression can be presented in a more convenient form:

$$y_{jn+1} = \sum_{i=0}^1 a_{ji} y_j(n) + \sum_{i=0}^1 b_{ji} y_{j-1}(n) + \sum_{i=0}^1 c_{ij} x_j(n-1) + \sigma \varepsilon_{jn} \quad (6)$$

The given approach to the development of mathematical models can be distributed to many continuous industrial processes.

To estimate unknown coefficients of the given model, identification method has been developed, that is known methods are not efficient in the cases of interferences correlation.

The task is set: on the basis of the data from the industrial object of continuous operation, to find such a mathematical model of this object, which approaches in the best way to the real object in the matter of certain criterion.

This task is a task of stochastic model identification taking into account interferences correlation, presented by the equation (5) /1-5/.

To calculate estimates of models parameters, such equations as Yule-Walker equations /6,7/, including distribution moments, which can be received in the following manner have been suggested.

We will multiply right and left parts of the equation (5) by Y_{n-k} and X_{n-k} at $k > 0$ and sum over all $n = 1, 2, \dots, N$. Passing to mathematical expectations at $M[Y_{n-k}\varepsilon_n] = 0$, we will receive the following equations:

$$R_{YY}(k) = (\theta + \lambda)R_{YY}(k+1) - \theta\lambda R_{YY}(k+2) + AR_{XY}(k+1) - A\lambda R_{XY}(k+2) \quad (7)$$

$$R_{XY}(k) = (\theta + \lambda)R_{XY}(k+1) - \theta\lambda R_{XY}(k+2) + AR_{XX}(k+1) - A\lambda R_{XX}(k+2) \quad (8)$$

The joint solution of any two of these equations allows to receive optimum estimates of model parameters.

It is not difficult to show that the method of least squares is a particular case of the suggested method at non-correlated noise. Estimates of model parameters by the method of least squares are received at joint solution of the chosen equations in a certain manner from the number of Yule-Walker equations in shear $k = 0$.

For statics model (1) Yule-Walker equations are given by:

$$(1 - \theta)R_{XY}(k) = AR_{XX}(k), \quad k \geq 0 \quad (9)$$

Here estimates of \hat{A} coefficients are received by the method of least squares, solving the equation (9) at $k = 0$. Relations for calculating estimates of dynamic model coefficient (2) are given by:

$$R_{YY}(k+1) = \theta R_{YY}(k) + AR_{XY}(k) \quad (10)$$

$$R_{XY}(k+1) = \theta R_{XY}(k) + AR_{XX}(k) \quad (11)$$

The identification quality will be estimated according to the value of mean-root-square error (MRQE) of the forecast of output variable of the state for one step at the given realization δ .

The value of MRQE of the filtration δ_{st} for some estimates of static system parameters can be expressed as the following:

$$\delta_{st.} = \frac{1}{N} \sum_{n=1}^N [y_n - \hat{A}x_n\tau]^2 = \hat{R}_{yy}(0) - 2\hat{A}\tau\hat{R}_{xy}(0) + A^2\tau^2\hat{R}_{xx}(0) \quad (12)$$

Estimates of forecast dispersion δ_{dyn} for the dynamic system are defined from the expression:

$$\begin{aligned}\hat{\delta}_{dyn.} &= \frac{1}{N} \sum_{n=1}^N [y_n - y_{n-1}\theta - \hat{A}x_{n-1}]^2 = \\ &= (1 + \theta^2)\hat{R}_{yy}(0) + 2\theta\hat{R}_{yy}(1) + 2\theta\hat{A}\hat{R}_{xy}(0) - 2\hat{A}\hat{R}_{xy}(1) + \hat{A}^2\hat{R}_{xx}(0)\end{aligned}\quad (13)$$

The value of mean-root-square error of δ forecast to estimate parameters for dynamic system taking into account interferences correlation can be expressed as the following:

$$\begin{aligned}\hat{\delta} &= \frac{1}{N} \sum_{n=1}^N [y_{n+1} - \hat{y}_{n+1}]^2 = \frac{1}{N} \sum_{n=1}^N [y_{n+1} - (\theta + \hat{\lambda})y_{n-1} - \hat{A}x_n + \hat{A}\hat{\lambda}x_{n-1}]^2 = \\ &= \varphi_1\hat{R}_{yy}(0) + \varphi_2\hat{R}_{yy}(1) + \varphi_3\hat{R}_{yy}(2) + \varphi_4\hat{R}_{yy}(-1) + \varphi_5\hat{R}_{xy}(0) + \\ &+ \varphi_6\hat{R}_{xy}(1) + \varphi_7\hat{R}_{xy}(2) + \varphi_8\hat{R}_{xx}(0) + \varphi_9\hat{R}_{xx}(1);\end{aligned}\quad (14)$$

or

$$\hat{\delta} = \sum_{\tau=-1}^2 \hat{R}_{yy}(\tau)\varphi_{\tau} + \sum_{\tau=0}^2 \hat{R}_{xy}(\tau)\varphi_{\tau} + \sum_{\tau=0}^1 \hat{R}_{xx}(\tau)\varphi_{\tau}$$

The results of coefficients calculations of two variants of models and criteria of identification have been shown in the Table 1 and 2.

Table 1. Parameter estimation A and error of prediction for models with uncorrelated hindrance

K	Statics		Dynamics	
	$A_{cr} \cdot 10^{12}$	$\delta_{cr.}$	$A_{дин.} \cdot 10^{10}$	$\delta_{дин.}$
0	0,07	1,65	1,23	1,058
1	0,67	1,74	1,78	1,069
2	1,33	2,06	1,50	1,061
3	1,76	2,39	1,66	1,066
4	2,18	2,81	1,57	1,063
5	2,01	2,62	1,18	1,059

Table 2. Estimated coefficients and error of prediction allowing for correlation of hindrance

$\hat{A} \cdot 10^{12}$	θ	Error of prediction δ
40,66	0,37	34,5
23,67	0,105	8,20
0,16	1,76	1,09
1,33	3,08	0,60
2,50	0,23	0,92

The analysis of the results shows that recording object dynamics allows to decrease forecast dispersion by 40-50%. Recording interferences correlation at the output of the object decreases forecast dispersion estimate by 60-70%. Therefore, the mathematical model of the polymerization process taking into account interferences correlation allows to receive the best forecast, that is it is more precise.

3. Conclusion

All Mathematical models of technological processes allowing to take into account the factors, influencing on conditions of production have been suggested.

The method of identifying mathematical models allowing to obtain from the object optimal estimate of parameters of industrial process according to data of normal use has been developed.

Researching opportunities of developing mathematical models of industrial processes of styrol polymerization allowed to identify the presence of certain factors while carrying out industrial processes in conditions of operating enterprise which don't enable to receive mathematical model, adequate to industrial process. In the article detailed analysis of mathematical models of reactors to manage bulk industrial reactors have been carried out. The methods of mathematical modeling of processes in industrial apparatus of reactor type with stirring device have been presented. Stochastic models with account of hindrance correlation in terms of Wall-Worker (Уола-Уокера) have been developed on the basis of dynamic models of reactors. Such kind of modeling method is presented as identification of model of industrial process. As polymerization process is carried out in reactors of continuous action, accounting correlation of hindrance is substantiated. Numerical experiments, showing efficiency of the presented method of identification have been carried out in the article.

The method of identifying mathematical models of chemical reactors of styrol polymerization in conditions of continuous operating industrial production and their identification allowing to carry out scale-up has been suggested. On the basis of researches of conditions of industrial polymerization of styrene the way of identification of stochastic model of process is offered. In a basis of a way Yule-Walker algorithms are put, allowing to consider correlated errors and to receive the best forecast of the basic characteristics of process.

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